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# High-Throughput Screening Platform for Solid Electrolytes

## Combining Hierarchical Ion-Transport Prediction Algorithms

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# 1 Main interface

## 1.1 Components of the main interface

Figure 1 shows the main interface of SPSE. The main interface consists of the following parts:

- Navigation bar:** “Home”, “Language switching”, “Search”, “Calculation”, “Upload”, “Sign up” and “Sign in” menus are placed on the navigation bar.
- Periodic table:** Click the symbol button to select an element symbol from the periodic table.
- Search options:** search options include the space group number, data source, article title, year, BVSE values, data ID, and elements. There is a logical relationship between elements: AND, OR, and NOT.

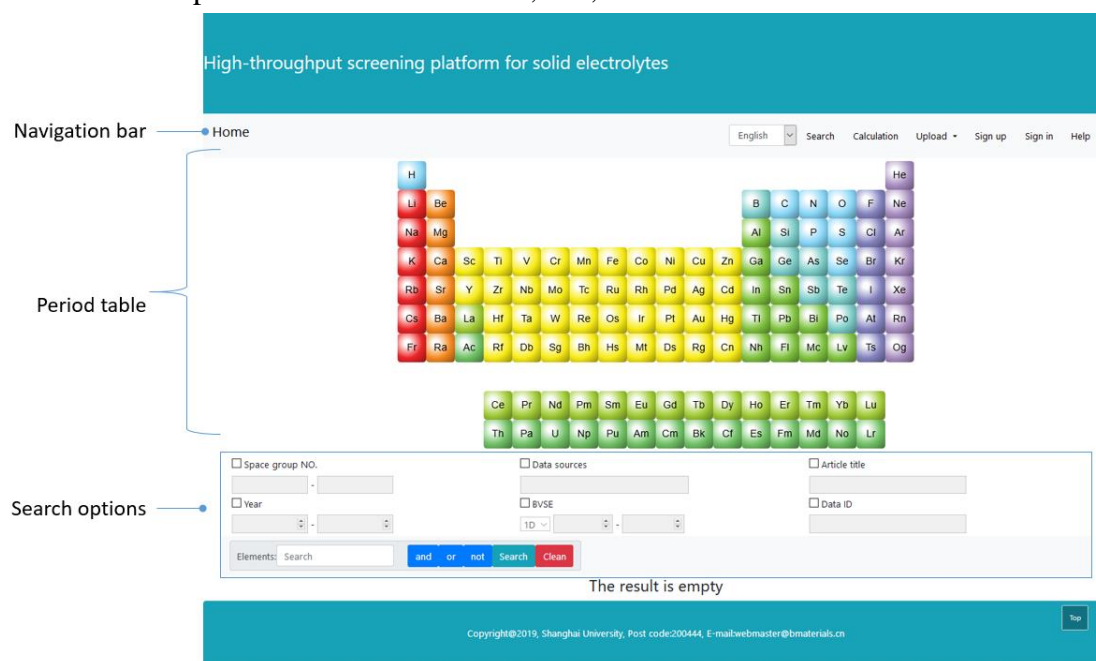


Fig. 1. Main interface-search page

## 1.2 Menus

- Home menu:** Jump to the main interface.
- Language switching menu:** Currently, “English” and “Chinese” languages are optional for the website.
- Search menu:** Jump to the search interface, also the main interface.
- Calculation menu:** Jump to the calculation interface.
- Upload menu:**
  - Document upload: Jump to the “Document upload” interface.

- CIF upload: Jump to the “CIF upload” interface.
- f) **Help menu:** Jump to the “Help” interface.
- g) **Sign up menu:** Jump to the “Sign up” interface to register a new user.
- h) **Sign in menu:** Jump to the “Sign in” interface to sign in.

### 1.3 Search results

There are 518 data, a total of 26 pages with  data per page.

<input type="checkbox"/> All	▲Data sources	▲ID	a	b	c	$\alpha$	$\beta$	$\gamma$	▲Chemical formula	▲Space group	▲Creation date	Details
<input type="checkbox"/>	icsd	12142	4.710	4.710	31.720	90.000	90.000	120.000	Li5NaSn4	R 3 m H	1980-01-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	54244	6.798	6.798	6.798	90.000	90.000	90.000	Li2NaSb	F m -3 m	2005-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	57410	6.798	6.798	6.798	90.000	90.000	90.000	Li2NaSb	F m -3 m	2005-04-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	61091	4.026	4.026	6.495	90.000	90.000	90.000	NaLiS	P 4/n m m S	1986-12-03	<a href="#">Details</a>
<input type="checkbox"/>	icsd	67274	7.740	4.624	8.406	90.000	90.000	90.000	NaLiTe	P n m a	1990-12-27	<a href="#">Details</a>
<input type="checkbox"/>	icsd	67359	7.174	4.249	7.716	90.000	90.000	90.000	LiNaSe	P n m a	1990-12-27	<a href="#">Details</a>
<input type="checkbox"/>	icsd	68069	17.972	3.788	10.299	90.000	90.000	90.000	Li3NaSi6	P n m a	1991-07-10	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92305	3.653	3.653	5.337	90.000	90.000	90.000	Li4Na2N2	I 4/m m m	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92306	5.265	5.265	5.265	90.000	90.000	90.000	Li4Na2N2	F m -3 m	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92307	3.698	6.365	4.600	90.000	90.000	90.000	Li4Na2N2	C m m m	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92308	3.650	3.650	4.600	90.000	90.000	120.000	Li2NaN	P 6/m m m	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92309	3.895	3.895	6.114	90.000	90.000	90.000	Li2Na4N2	P 4/n m m Z	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92310	4.000	4.000	4.200	90.000	90.000	120.000	LiNa2N	P 6/m m m	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92311	3.652	3.652	5.436	90.000	90.000	90.000	Li3Na3N2	P -4 m 2	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92312	3.854	3.676	6.320	90.000	90.310	90.000	Li3Na3N2	P 1 m 1	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92313	3.965	3.965	5.504	90.000	90.000	90.000	Li5NaN2	P 4/m m m	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92314	4.280	3.860	7.827	90.000	121.710	90.000	Li5NaN2	P 1 m 1	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92315	6.731	5.944	6.383	90.000	91.180	90.000	LiNa5N2	C 1 2 1	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	92316	6.570	4.056	3.729	89.480	90.530	88.840	LiNa5N2	P 1	2002-10-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	103784	24.666	15.974	45.271	90.000	90.000	90.000	Ga19.56Li3Na5	F m m m	2004-10-01	<a href="#">Details</a>

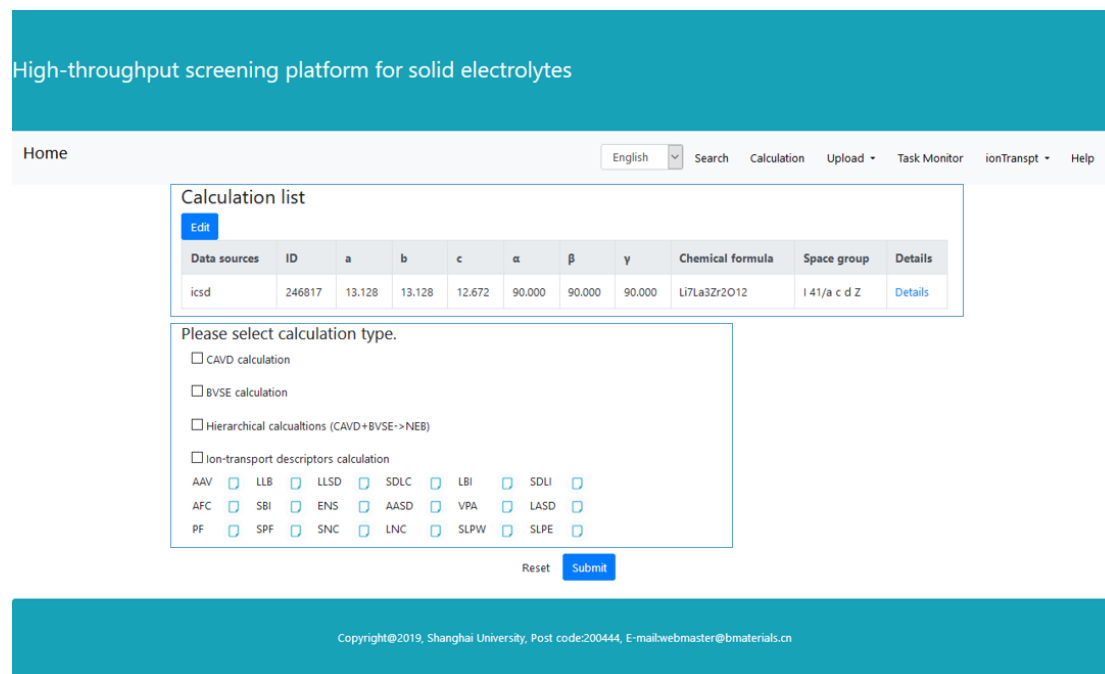
>
 >>

**Fig. 2.** Results of a “Li & Na” search.

For instance, 518 compounds containing Li and Na are obtained by searching for “Li & Na” (Figure 2); by default, 20 data displayed on one page and user can change the amounts. The search results provide common information about the structure, including the data source, data identifier, lattice constant lengths, lattice constant angles, chemical formula, space group, and creation date. More details about the structure can be obtained by clicking “Details” to access the details page. Additionally, data can be downloaded in batches for analysis by clicking the “Download CIFs” or “Download computational data” button. The search page allows users to select the structure(s) of interest and click the “Add to calculation list” button to jump to the Materials Calculation page.

## 2 Materials calculation interface

The materials calculation interface consists of two parts: calculation list and calculation type. Currently, CAVD, BVSE, ion-transport descriptor, and hierarchical (CAVD + BVSE → NEB) calculations are possible (Figure 3).



High-throughput screening platform for solid electrolytes

Home English Search Calculation Upload Task Monitor ionTranspt Help

Calculation list

Edit

Data sources	ID	a	b	c	$\alpha$	$\beta$	$\gamma$	Chemical formula	Space group	Details
icsd	246817	13.128	13.128	12.672	90.000	90.000	90.000	Li7La3Zr2O12	I 41/a c d Z	<a href="#">Details</a>

Please select calculation type.

CAVD calculation

BVSE calculation

Hierarchical calculations (CAVD+BVSE→NEB)

Ion-transport descriptors calculation

AAV  LLB  LLSD  SDLC  LBI  SDU

AFC  SBI  ENS  AASD  VPA  LASD

PF  SPF  SNC  LNC  SLPW  SLPE

Reset Submit

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**Fig. 3.** Materials calculation interface

CAVD calculation

Mobile ion

Li

Radius?  YES  NO

Minimum radius of bottleneck/void

0.5

Maximal radius of bottleneck/void

10

**Fig. 4.** Parameter setting for CAVD calculation.

BVSE calculation

Mobile ion

Li

Valence

1

Grid resolution

0.1

**Fig. 5.** Parameter setting for BVSE calculation.

Hierarchical calculations (CAVD+BVSE->NEB)

**Parameter settings of CAVD+BVSE**

Mobile ion

Valence

Grid resolution

Radius?  YES  NO

Minimum radius of bottleneck/void

Maximal radius of bottleneck/void

**Screening parameters of CAVD+BVSE**

Screening by CAVD radius  
 -


Screening by BVSE value  
  -

**Parameter settings of NEB**

VASP script

Due to the limitation of computing resources, high-precision computing is not provided for the time being.

**Fig. 6.** Parameter setting for hierarchical calculations.

- a) Crystal structure analysis by Voronoi decomposition (CAVD): the screening radii of bottlenecks and voids have default values, and the required parameter is the type of mobile ion (Li, Na, Mg, Al, Ag, Zn, Cu, F and O are optional).
- b) Bond-valence site energy (BVSE): Similarly, the type and valence of the mobile ion are required for BVSE and hierarchical calculations, and the grid resolution is an optional parameter.
- c) Ion-transport descriptor: No parameters are required for the calculation of ion-transport descriptors. The picture “” after the descriptor can be clicked to view the formulas of the 22 ion-transport descriptors.

## 3 Detail interface

The detail of structure is show in the detail interface. It contain the structure visualization (Figure 7) and structure data.

### 3.1 Components of structure visualization

- a) Tools in the style panel:
  - Supercell: View in 2\*2\*2 supercell, or 10Å box, or reset in unit cell.
  - Visulation: View in Ball-and-stick, space-filling, or polyhedra.
  - Axis: View along the a, b, or c axis.
  - Rotation: Rotation the structure.
  - Labels: Lable the atoms in structure.
  - Background: View in the black background.

b) Tools in save panel:

Save the CIF file, or state, JPG, PNG or PNG+Jmol.

c) The instructions of JSmol panel are show in Figure 8.

Structure — icسد\_246817: Li7La3Zr2O12

Jsmol instructions

Instructions

$HM=1$  41/a c d z  
 $a=13.128\text{\AA}$   
 $b=13.128\text{\AA}$   
 $c=12.672\text{\AA}$   
 $\alpha=90.000^\circ$   
 $\beta=90.000^\circ$   
 $\gamma=90.000^\circ$

Jsmol panel

Save panel

Save: CIF file STATE JPG PNG PNG+JSmol

Style panel

Supercell:

2\*2\*2

10Å box

reset

Visualization:

Ball-and-Stick

Space-filling

Polyhedra

Rotation

Labels

Background

axis:

a b c

**Fig. 7.** Structure visualization.

Instructions

To rotate the model, just put the mouse pointer over the Jmol panel and drag (move the mouse while you hold its button pressed down).In this way, the model rotates around the X (horizontal) and Y (vertical) axes; if you need to rotate around Z axis (perpendicular to screen), hold down the Shift key while dragging horizontally.

To zoom in (closer) or zoom out (farther), so changing the model's apparent size, click on the Jmol panel and then use the mouse wheel, or hold the Shift key while dragging vertically.

To measure a distance (such as a bond length), double-click on an atom; when you move the pointer, a dotted line will be shown, and when it is positioned on a second atom the distance will be displayed. If you double-click on the second atom, the measurement will be permanently displayed.

To measure an angle, double-click on an atom; move the pointer to the second atom and single-click; then move it to the third atom and the angle will be displayed. If you double-click on the third atom, the measurement will be permanently displayed.

The set of measurements may be hidden, shown again, permanently deleted or looked up in a list by means of the Measurements entry in the Jmol menu.

**Fig. 8.** JSmol instruction.

### 3.2 Components of structure data

- structure information (Figure 9)
- computational data (Figure 10)
  - CAVD calculation data;
  - BVSE calculation data;
  - Ionic migration path;
  - Ion-transport descriptor;

## Crystal structure

### Lattice constant

a	b	c	$\alpha$	$\beta$	$\gamma$	volume	z	refine ls r factor all
13.1279	13.1279	12.6715	90.0	90.0	90.0	2183.82	8	0.0076

### Chemical formula

Chemical name systematic	Chemical name common	Chemical formula	Chemical formula sum
Lithium Lanthanum Zirconium Oxide (7/3/2/12)	None	Li7La3Zr2O12	La3 Li7 O12 Zr2

### Space group

Space group NO.	Space group	Hall	symmetry cell setting
142	I 41/a c d Z	None	None

### Valence

Atomic type	Valence
La3+	3
Li1+	1
O2-	-2
Zr4+	4

### Atomic sites

Label	Atomic type	Wyckoff	X	Y	Z	Occupancy	Symmetry
La1	La3+	b	0	0.25	0.125	1.0	8
La2	La3+	e	0.127	0	0.25	1.0	16
Zr1	Zr4+	c	0	0	0	1.0	16
Li1	Li1+	a	0	0.25	0.375	1.0	8
Li2	Li1+	f	0.1797	0.4297	0.125	1.0	16
Li3	Li1+	g	0.0806	0.0857	0.8041	1.0	32
O1	O2-	g	-0.0338	0.0548	0.1524	1.0	32
O2	O2-	g	0.0541	0.8529	0.5338	1.0	32
O3	O2-	g	0.1496	0.0276	0.4464	1.0	32

### Data sources

Data sources	ID	Article title	Article author
icsd	246817	Synthesis and structure analysis of tetragonal Li7...	Awaka, J.;Kijima, N.;Hayakawa, H.;Akimoto, J.

### Date

Creation date	Update date
2010/02/01	2010/02/01

### Citations

ID	Year	First page	Last page	Journal volume	ASTM_id	Journal abbrev
primary	2009	2046	2052	182	JSSCBI	Journal of Solid State Chemistry

**Fig. 9.** Structure information.

## Data from calculations or articles

### CAVD data

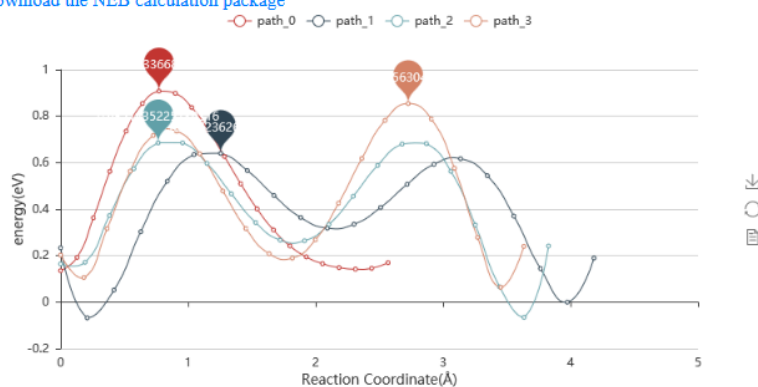
Rf_a	Rf_b	Rf_c	Channel_threshold	con_a	con_b	con_c	Original network	Geometric channel
0.56	0.56	0.56	0.5	True	True	True	<a href="#">.net.VASP</a>	<a href="#">.net.VASP</a>

### BVSE data

Mobile ion	BVSE_1d(eV)	BVSE_2d(eV)	BVSE_3d(eV)	BVEL_1d(eV)	BVEL_2d(eV)	BVEL_3d(eV)	GRD file
Li	0.693359375	0.869140625	0.87890625	0.712890625	0.87890625	0.87890625	<a href="#">Download</a>

### Ionic migration path

[Download the NEB calculation package](#)



### Ion-transport descriptors calculation

llb	llsd	sdlc	lbi	sqli	afc	sbi	ens	aasd	vpa	lasd	pf	aav	spf	snc	lnc	slpw	slpe
5.71	2.57	0.89	1.48	1.15	11.0	1.08	2.78	3.18	22.75	1.9	0.83	0.61	11.37	20.71	21.71	0.45	1.54

**Fig. 10.** Calculation data.

## 3.3 Download computational data

The BVSE data, CAVD data and ion migration paths can be downloaded in the structure details interface (see Fig. 10). The GRD file and NEB calculation package of  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  are downloaded and explained here.

- (1) The GRD file is opened with VESTA to visualize migration path. The VESTA settings are shown in Fig 11 and visualization is shown in Fig 12.



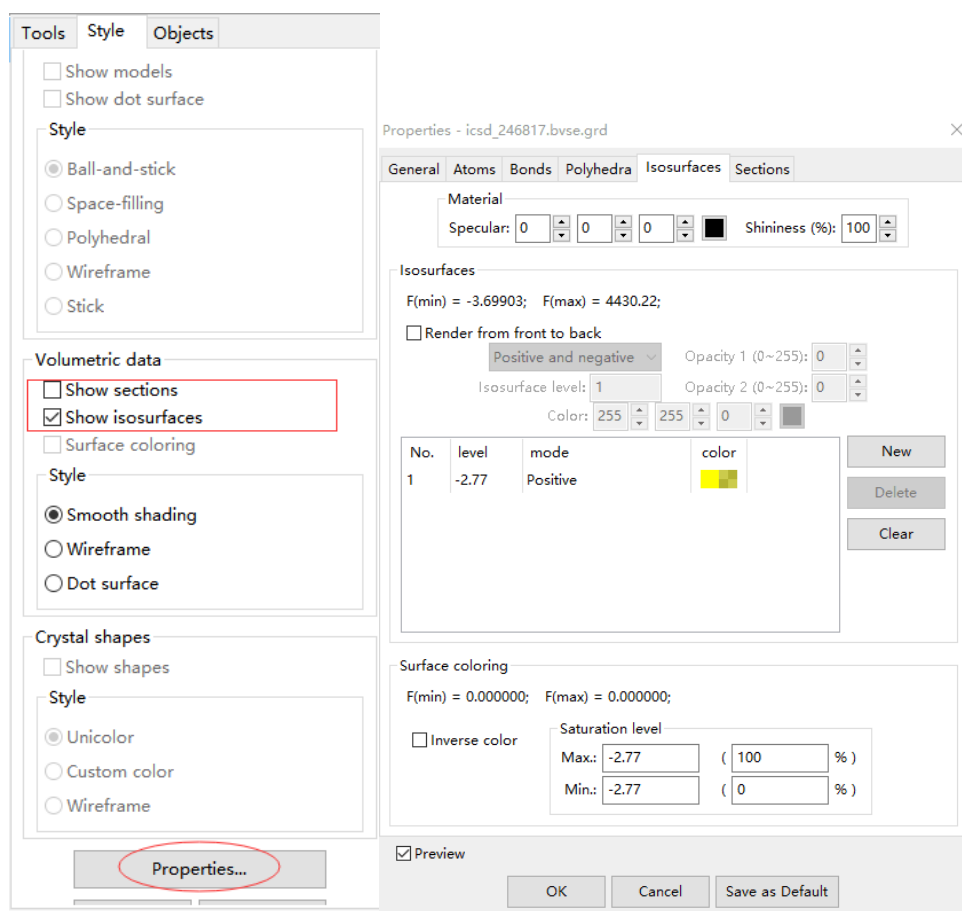


Fig. 11. VESTA settings.

icسد\_246817.bvse.grd

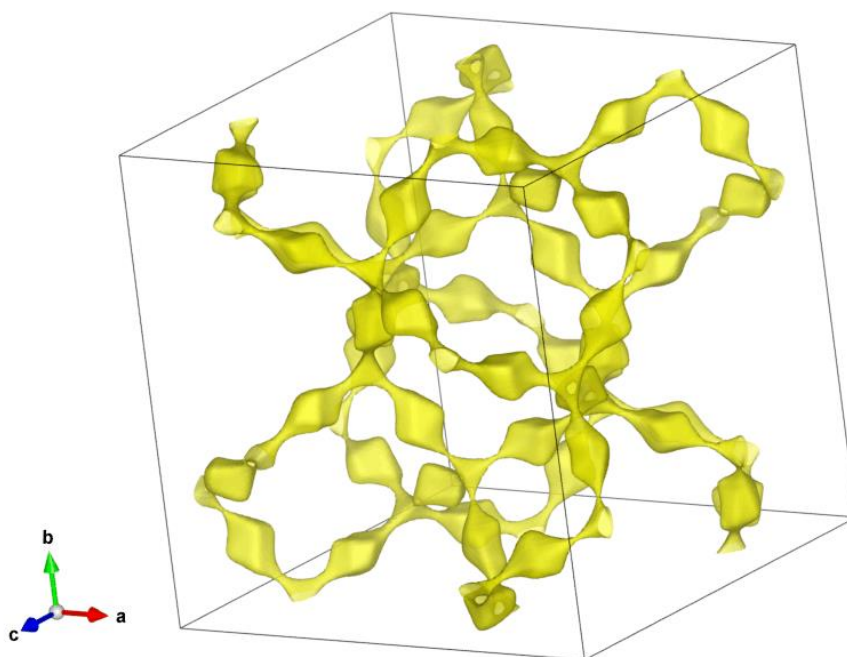
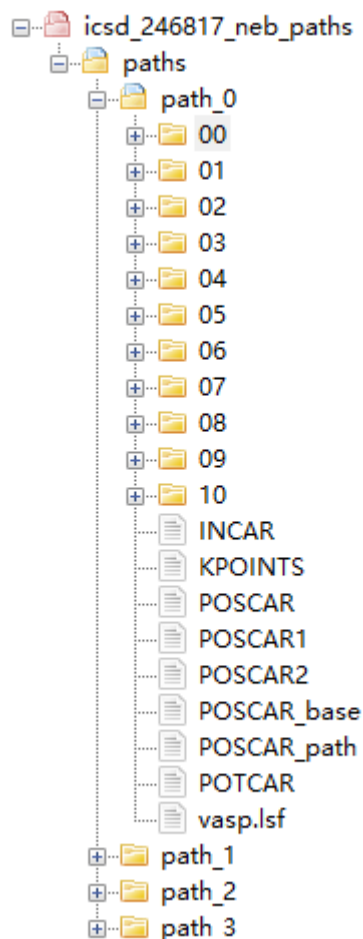


Fig. 12. Migration path of  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ .

- (2) The NEB calculation package is a zip file obtained by hierarchical calculation, which contains all the input files required by NEB VASP calculation of the non-equivalent migration paths in the structure. Taking  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  as an example, the NEB calculation data of four non-equivalent paths are included. Among them, INCAR, KPOINTS and POTCAR are input files for VASP to calculate NEB. The decompressed directory is as follows:



**Fig. 13.** NEB calculation package.

- (3) The POSCAR\_path file can be visualized with VESTA:

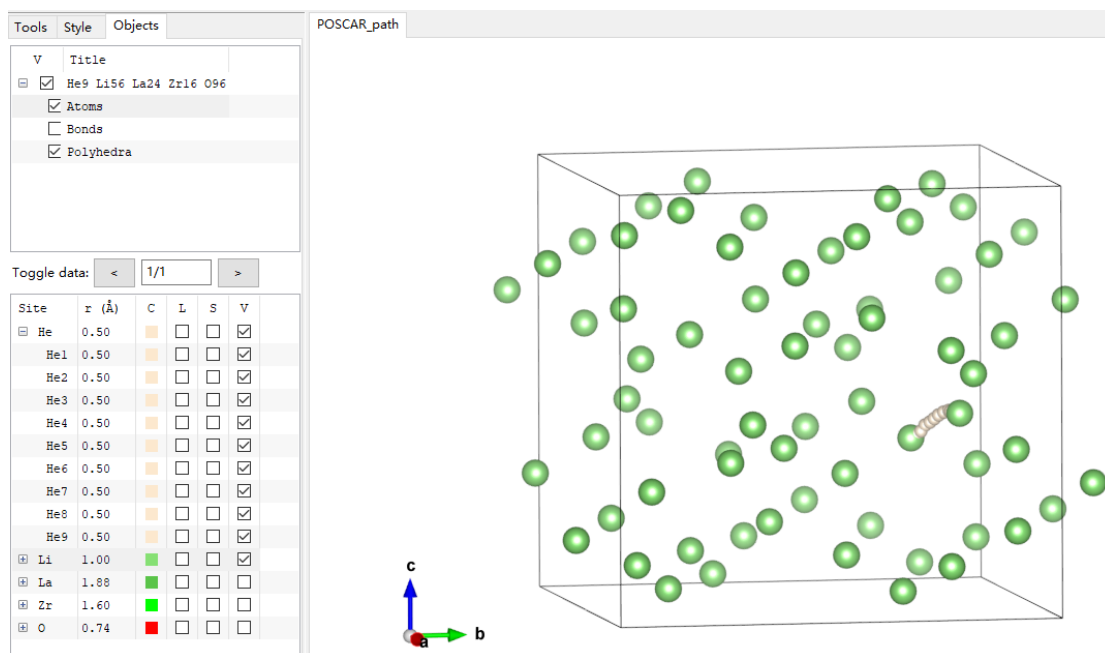


Fig. 14. Visualization of POSCAR\_path file.

## 4 CIF upload interface

In consideration of the demand for additional structures, a Data Upload option is provided for users to upload CIF(s). Users can upload CIF file(s) or .zip file(s) containing CIF files.



Fig. 15. CIF upload interface.

## 5 Task monitor

Users can query the states of their submitted tasks using Task Monitor (the states include READY, RUNNING, COMPLETED, FIZZLED, etc.). It shows all tasks submitted by current user. Click “Details” of one task to view the structures of the submission. For each structure, the execution task ID represents the specific task id of the calculation task, and click the id to see the status of current calculation task.

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Home English Search Calculation Upload Task Monitor ionTranspt Help

Task ID	Creation date	Submission status	Submission time	Submitter	Task details
5d517c6e26e8a9135f640b2d	Aug. 12, 2019, 10:49 p.m.	True	Aug. 12, 2019, 10:49 p.m.	ionTranspt	<a href="#">Details</a>
5d516c35a946eb966ff1cc07	Aug. 12, 2019, 10:39 p.m.	True	Aug. 12, 2019, 10:39 p.m.	ionTranspt	<a href="#">Details</a>
5d5149afa946eb966ff1cc03	Aug. 12, 2019, 7:12 p.m.	True	Aug. 12, 2019, 7:12 p.m.	ionTranspt	<a href="#">Details</a>
5d510436a8829100bdbde59d	Aug. 12, 2019, 7:12 p.m.	True	Aug. 12, 2019, 7:12 p.m.	ionTranspt	<a href="#">Details</a>
5d50ffdc8829100bdbde46b	Aug. 12, 2019, 1:57 p.m.	True	Aug. 12, 2019, 1:58 p.m.	ionTranspt	<a href="#">Details</a>
5d3e52ab9caa716185b68436	July 29, 2019, 9:58 a.m.	True	July 29, 2019, 9:58 a.m.	ionTranspt	<a href="#">Details</a>
5d3e40639caa716185b68433	July 29, 2019, 8:40 a.m.	True	July 29, 2019, 8:40 a.m.	ionTranspt	<a href="#">Details</a>

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**Fig. 16.** All tasks.

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Home English Search Calculation Upload Task Monitor ionTranspt Help

Task details

Task ID	Creation date	Submission status	Submission time	Submitter
5d517c6e26e8a9135f640b2d	Aug. 12, 2019, 2:49 p.m.	True	Aug. 12, 2019, 2:49 p.m.	ionTranspt

Structure information

Data sources	ID	a	b	c	$\alpha$	$\beta$	$\gamma$	Chemical formula	Execution task ID	Details
icsd	246817	13.128	13.128	12.672	90.000	90.000	90.000	Li7La3Zr2O12	3378	<a href="#">Details</a>

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**Fig. 17.** Task details.

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Home English Search Calculation Upload Task Monitor ionTranspt Help

Details of calculation task

Execution task ID  
2855

Task name  
cavd\_icsd\_100004\_ionTranspt\_6d8adc9a-b199-11e9-8f2b-f80f41f69e0b

Submitter  
ionTranspt

Status  
COMPLETED

Runtime  
4.59256

Parameter settings  
{'structid': '5ce3b21ad20cae08c0251b21', 'origin': 'icsd', 'origin\_id': 100004, 'transport\_ion': 'Li', 'rad\_flag': True, 'minRad': 0.5, 'maxRad': 10.0}

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**Fig. 18.** Details of calculation task.

## 6 User interface

In order to enjoy complete functions of SPSE, user should sign in the website. If you don't have an account, you can go to the "Sign up" interface to create a new account. There are five options for users:

- Sign up;
- Sign in;
- Profile;
- Sign out;
- Password Reset;
- Change password;
- E-mail Addresses.

(a) **Sign Up**  
 Already have an account? Then please [sign in](#).  
 E-mail\*  
  
 Username\*  
  
 First name  
  
 Last name  
  
 Organization  
  
 City  
  
 Country  
  
 Password\*  
  
 Password (again)\*

(b) **Sign In**  
 If you have not created an account yet, then please [sign up](#) first.  
 Login\*  
  
 Password\*  
  
 Remember Me  
[Forgot Password?](#)

(c) Welcome, ionTranspt.  
**My Profile**  

- First Name: I
- Last Name: TP
- Email: webmaster@bmaterials.cn
- Organization: SHU
- Country: China
- City: Shang hai

(d) **Sign Out**  
 Are you sure you want to sign out?

(e) **Password Reset**  
**Note:** you are already logged in as cst.  
 Forgotten your password? Enter your e-mail address below, and we'll send you an e-mail allowing you to reset it.  
 E-mail:   
  
 Please contact us if you have any trouble resetting your password.

(f) **Change Password**  
 Current Password:   
 New Password:   
 New Password (again):

(g) **E-mail Addresses**  
 The following e-mail addresses are associated with your account:  
 webmaster@bmaterials.cn Unverified Primary  
    
**Add E-mail Address**  
 E-mail:

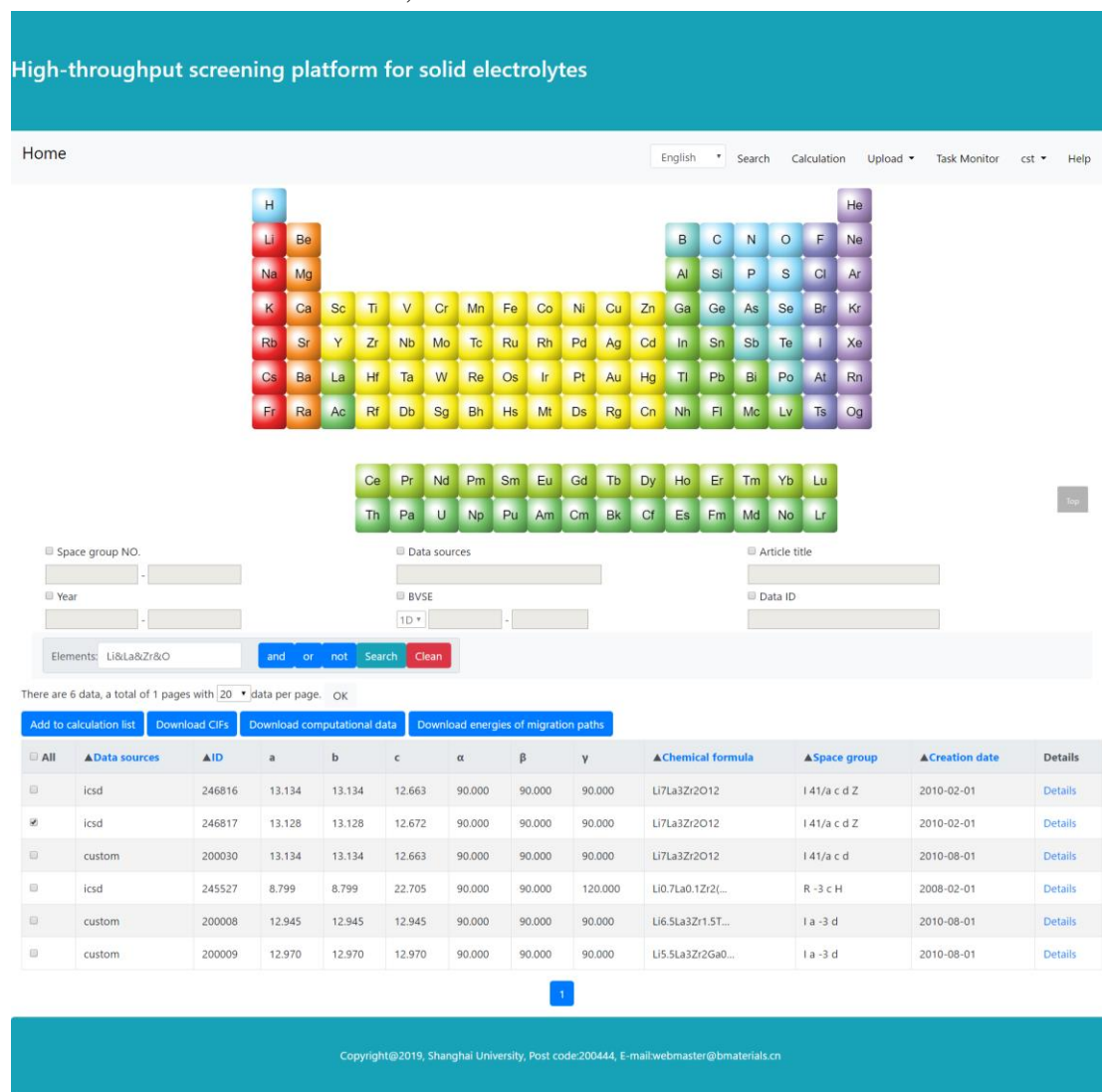
Fig. 19. Sign up interface.

## 7 Example

### 7.1 Enter the main interface

- Click the elements "Li, La, Zr and O" on the period table, and the click the "search" button;

- b) Select the structure  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) whose ID is 246817, and click “add to the calculation list” button;



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Home English Search Calculation Upload Task Monitor cst Help

Space group NO.  -   
 Year  -   
 Data sources   
 BVSE  -   
 Article title   
 Data ID

Elements: Li&La&Zr&O and or not Search Clean

There are 6 data, a total of 1 pages with 20 data per page. OK

[Add to calculation list](#) [Download CIFs](#) [Download computational data](#) [Download energies of migration paths](#)

All	Data sources	ID	a	b	c	$\alpha$	$\beta$	$\gamma$	Chemical formula	Space group	Creation date	Details
<input type="checkbox"/>	icsd	246816	13.134	13.134	12.663	90.000	90.000	90.000	$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	I 41/a c d Z	2010-02-01	<a href="#">Details</a>
<input checked="" type="checkbox"/>	icsd	246817	13.128	13.128	12.672	90.000	90.000	90.000	$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	I 41/a c d Z	2010-02-01	<a href="#">Details</a>
<input type="checkbox"/>	custom	200030	13.134	13.134	12.663	90.000	90.000	90.000	$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	I 41/a c d	2010-08-01	<a href="#">Details</a>
<input type="checkbox"/>	icsd	245527	8.799	8.799	22.705	90.000	90.000	120.000	$\text{Li}_0.7\text{La}_0.1\text{Zr}_2(\dots)$	R -3 c H	2008-02-01	<a href="#">Details</a>
<input type="checkbox"/>	custom	200008	12.945	12.945	12.945	90.000	90.000	90.000	$\text{Li}_6.5\text{La}_3\text{Zr}_1.5\text{T}\dots$	I a -3 d	2010-08-01	<a href="#">Details</a>
<input type="checkbox"/>	custom	200009	12.970	12.970	12.970	90.000	90.000	90.000	$\text{Li}_5.5\text{La}_3\text{Zr}_2\text{Ga}_0\dots$	I a -3 d	2010-08-01	<a href="#">Details</a>

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Fig. 20. Select structure and add it into the calculation list.

## 7.2 Enter the calculation interface

- a) Jump to the prompt interface and click the “Calculation” button on the navigation bar;



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Add success!

OK

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Fig. 21. Add success.

- b) Select “CAVD calculation”, “BVSE calculation” and “Hierarchical calculation”. The parameters are default values and click “submit” button.

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### Calculation list

[Edit](#)

Data sources	ID	a	b	c	$\alpha$	$\beta$	$\gamma$	Chemical formula	Space group	Details
icsd	246817	13.128	13.128	12.672	90.000	90.000	90.000	Li7La3Zr2O12	I 41/a c d Z	<a href="#">Details</a>

Please select calculation type.

CAVD calculation

Mobile ion

Radius?  YES  NO

Minimum radius of bottleneck/void

Maximal radius of bottleneck/void

BVSE calculation

Mobile ion

Valence

Grid resolution

Multi-precision calculations (CAVD+BVSE->NEB)

#### Parameter settings of CAVD+BVSE

Mobile ion

Valence

Grid resolution

Radius?  YES  NO

Minimum radius of bottleneck/void

Maximal radius of bottleneck/void

#### Screening parameters of CAVD+BVSE

Screening by CAVD radius  
 -

Screening by BVSE value  
 -  -

#### Parameter settings of NEB

VASP script

Due to the limitation of computing resources, high-precision computing is not provided for the time being.

Ion-transport descriptors calculation

AAV  LLB  LLS  SDLC  LBI  SDLI

AFC  SBI  ENS  AASD  VPA  LASD

PF  SPF  SNC  LNC  SLPW  SLPE

Reset [Submit](#)

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Fig. 22. Calculation interface.

### 7.3 Enter the “Task monitor” interface

- a) Jump to the prompt interface and click the “Task monitor” button on the navigation bar;

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Asia/Shanghai

Task ID	Creation date	Submission status	Submission time	Submitter	Task details
5d517fb755ef038e33d91fce	Aug. 12, 2019, 11:03 p.m.	True	Aug. 12, 2019, 11:06 p.m.	cst	<a href="#">Details</a>
5d503b5f3a91fca86e8c1c3b	Aug. 11, 2019, 11:59 p.m.	True	Aug. 11, 2019, 11:59 p.m.	cst	<a href="#">Details</a>
5d4fc62c47d884b781a281eb	Aug. 11, 2019, 3:39 p.m.	True	Aug. 11, 2019, 3:40 p.m.	cst	<a href="#">Details</a>
5d4bdf8db33eda835d4b7e8f	Aug. 8, 2019, 4:38 p.m.	True	Aug. 8, 2019, 5:02 p.m.	cst	<a href="#">Details</a>
5d4bcffda90f953f5234bf7f	Aug. 8, 2019, 3:32 p.m.	True	Aug. 8, 2019, 3:32 p.m.	cst	<a href="#">Details</a>
5d4adcccd38d61149ad473cac	Aug. 7, 2019, 10:14 p.m.	True	Aug. 7, 2019, 10:14 p.m.	cst	<a href="#">Details</a>
5d4adb838d61149ad473ca7	Aug. 7, 2019, 10:11 p.m.	True	Aug. 7, 2019, 10:11 p.m.	cst	<a href="#">Details</a>
5d4adb3609ba18890a74f848	Aug. 7, 2019, 10:07 p.m.	True	Aug. 7, 2019, 10:08 p.m.	cst	<a href="#">Details</a>
5d428b2142495b83040b2cee	Aug. 7, 2019, 10:04 p.m.	True	Aug. 7, 2019, 10:05 p.m.	cst	<a href="#">Details</a>
5d4148395fce6168a587601f	July 31, 2019, 4:42 p.m.	True	July 31, 2019, 4:45 p.m.	cst	<a href="#">Details</a>

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**Fig. 23.** All tasks.

- b) Click the detail of the latest submitted task (such as the submission time is 2019/7/23 00:38):
- c) Click the one of the execution task IDs to view the detail of task.

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任务详情

Task ID	Creation date	Submission status	Submission time	Submitter
5d517fb755ef038e33d91fce	Aug. 12, 2019, 3:03 p.m.	True	Aug. 12, 2019, 3:06 p.m.	cst

结构信息

Data sources	ID	a	b	c	$\alpha$	$\beta$	$\gamma$	Chemical formula	Execution task ID	Details
icsd	246817	13.128	13.128	12.672	90.000	90.000	90.000	Li7La3Zr2O12	3379 3380 3381	<a href="#">Details</a>

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**Fig. 24.** Task details.



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**Details of calculation task**

Execution task ID  
3379

Task name  
bvs\_icsd\_246817\_cst\_d15993a4-bd12-11e9-865b-f80f41f69e0b

Submitter  
cst

Status  
COMPLETED

Runtime  
4037.93898

Parameter settings  
{'structid': '5ac3613c9a98c38f50fdeadf', 'origin': 'icsd', 'origin\_id': 246817, 'transport\_ion': 'Li', 'valence': 1, 'resolution': 0.1}

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**Fig. 25.** Details of BVSE calculation task.

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**Details of calculation task**

Execution task ID  
3380

Task name  
cbNeb\_icsd\_246817\_cst\_d1678072-bd12-11e9-865b-f80f41f69e0b

Submitter  
cst

Status  
COMPLETED

Runtime  
100.941357

Parameter settings  
{'structid': '5ac3613c9a98c38f50fdeadf', 'origin': 'icsd', 'origin\_id': 246817, 'transport\_ion': 'Li', 'valence': 1, 'resolution': 0.1, 'rad\_flag': True, 'minRad': 0.5, 'maxRad': 10.0, 'cavd\_value1': 0.5, 'cavd\_value2': 1.0, 'bvse\_key': 'bvse\_1d', 'bvse\_value1': 0.0, 'bvse\_value2': 1.2}

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**Fig. 26.** Details of hierarchical calculation task.

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**Details of calculation task**

Execution task ID  
3381

Task name  
cavd\_icsd\_246817\_cst\_d171b542-bd12-11e9-865b-f80f41f69e0b

Submitter  
cst

Status  
COMPLETED

Runtime  
27.096178

Parameter settings  
{'structid': '5ac3613c9a98c38f50fdeadf', 'origin': 'icsd', 'origin\_id': 246817, 'transport\_ion': 'Li', 'rad\_flag': True, 'minRad': 0.5, 'maxRad': 10.0}

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**Fig. 27.** Details of CAVD calculation task.